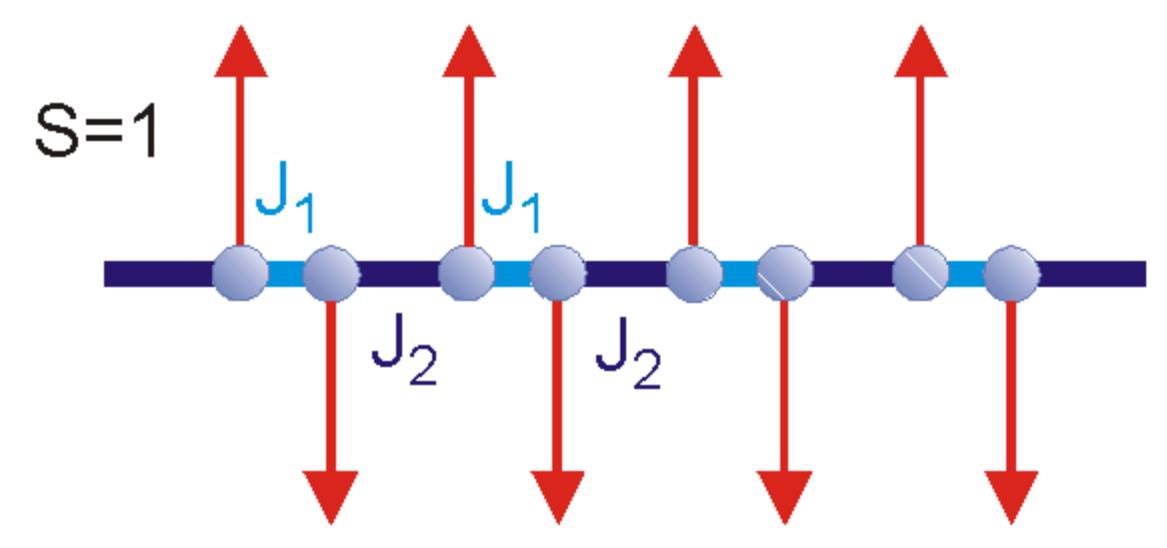


# Dimer gap vs. Haldane gap in S=1 chains

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## Phase diagram of S=1 bond-alternating chains



$$\hat{H} = \sum_j [J_1 \vec{S}_{2j}\vec{S}_{2j+1} + J_2 \vec{S}_{2j+1}\vec{S}_{2j+2} - g\mu_B h S_j^z]$$

• Neel order

$$O_{\text{Neel}}^\alpha = \lim_{|i-j| \rightarrow \infty} \langle S_i^\alpha (-1)^{i-j} S_j^\alpha \rangle$$

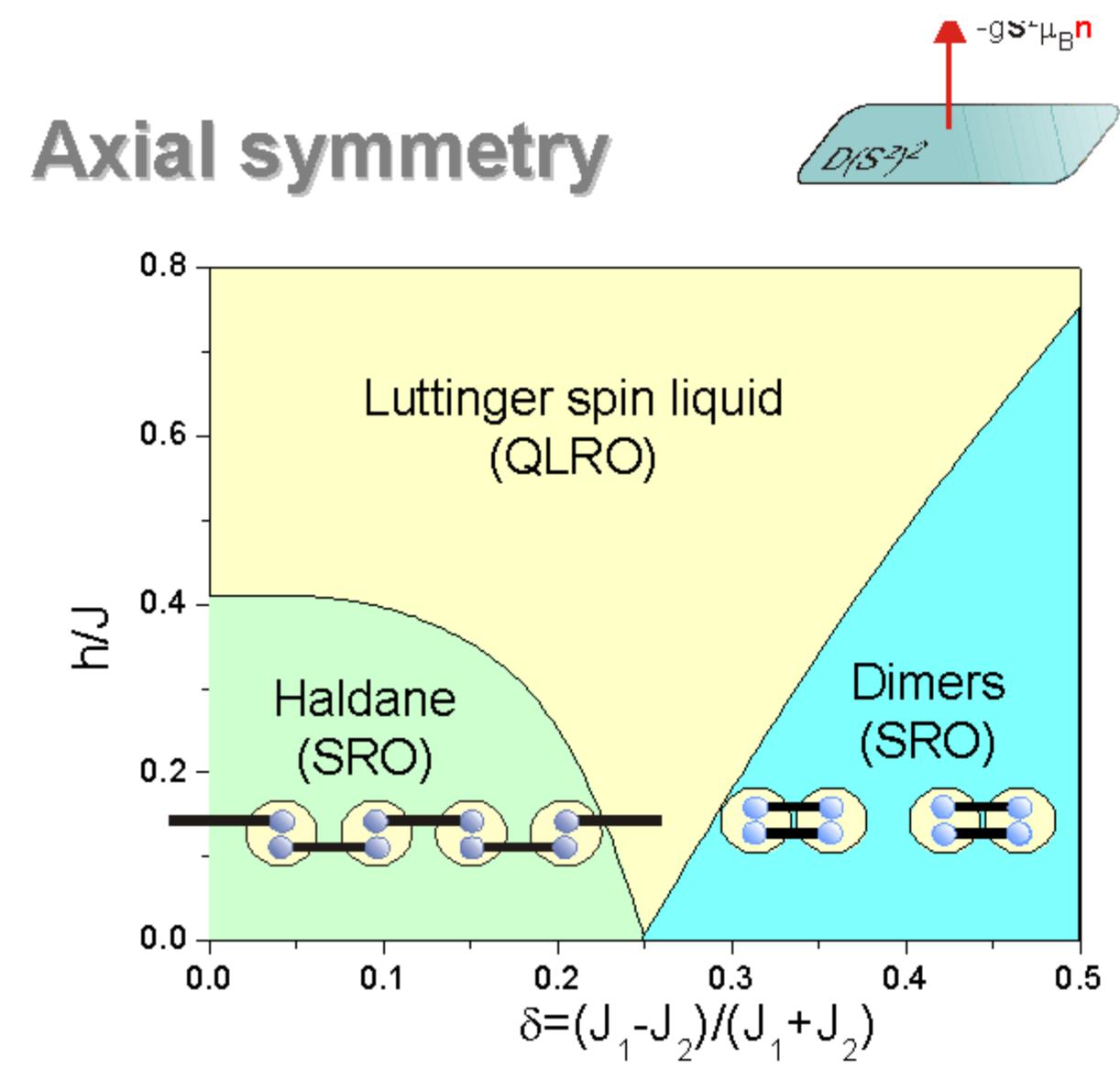
- local (pair) correlations
- directly observable

• String order

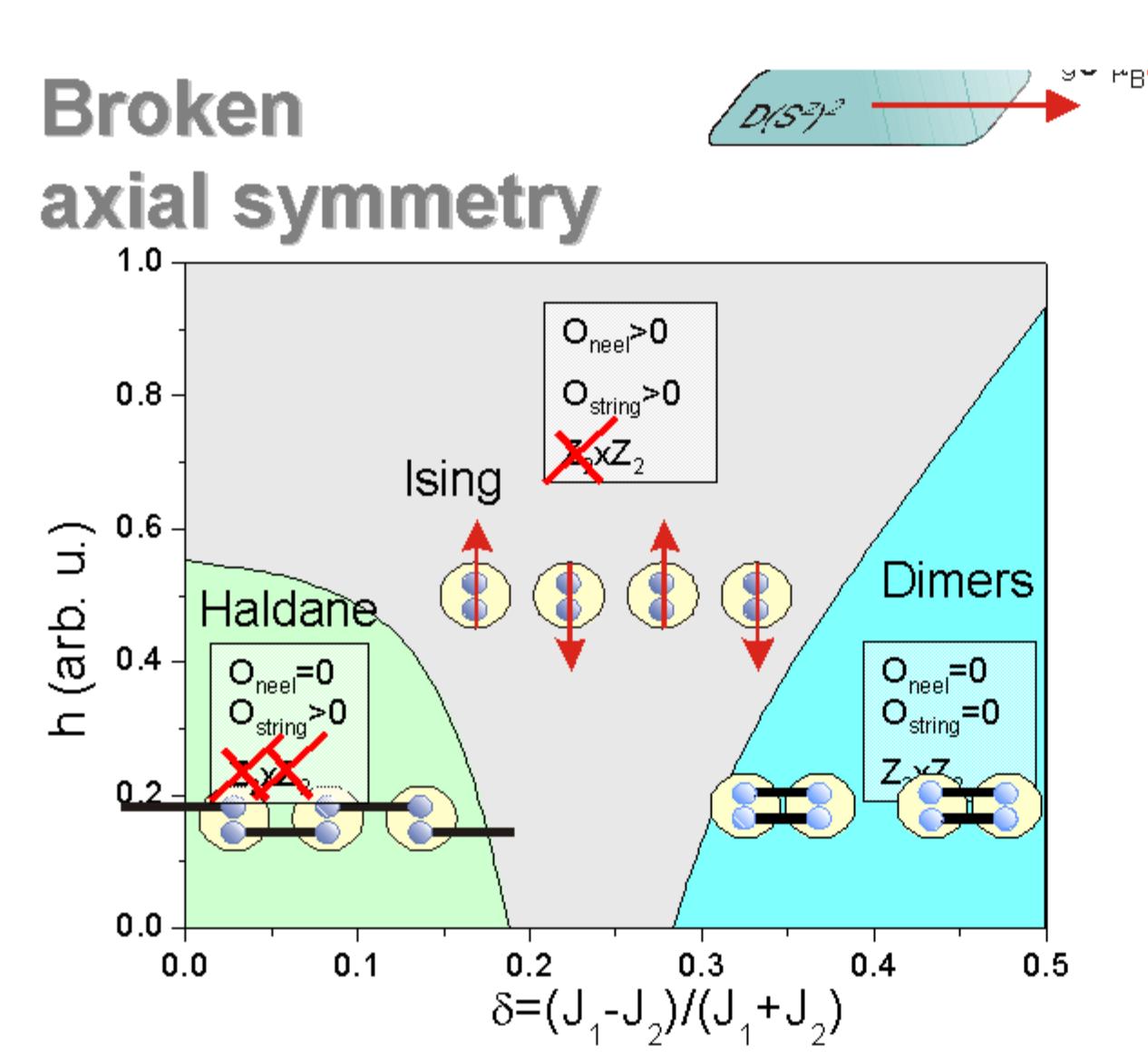
$$O_{\text{string}}^\alpha = \lim_{|i-j| \rightarrow \infty} \left\langle S_i^\alpha \exp\left[i\pi \sum_{k=i+1}^{j-1} S_k^\alpha\right] S_j^\alpha \right\rangle$$

- topological, non-local
- not observable

### Axial symmetry



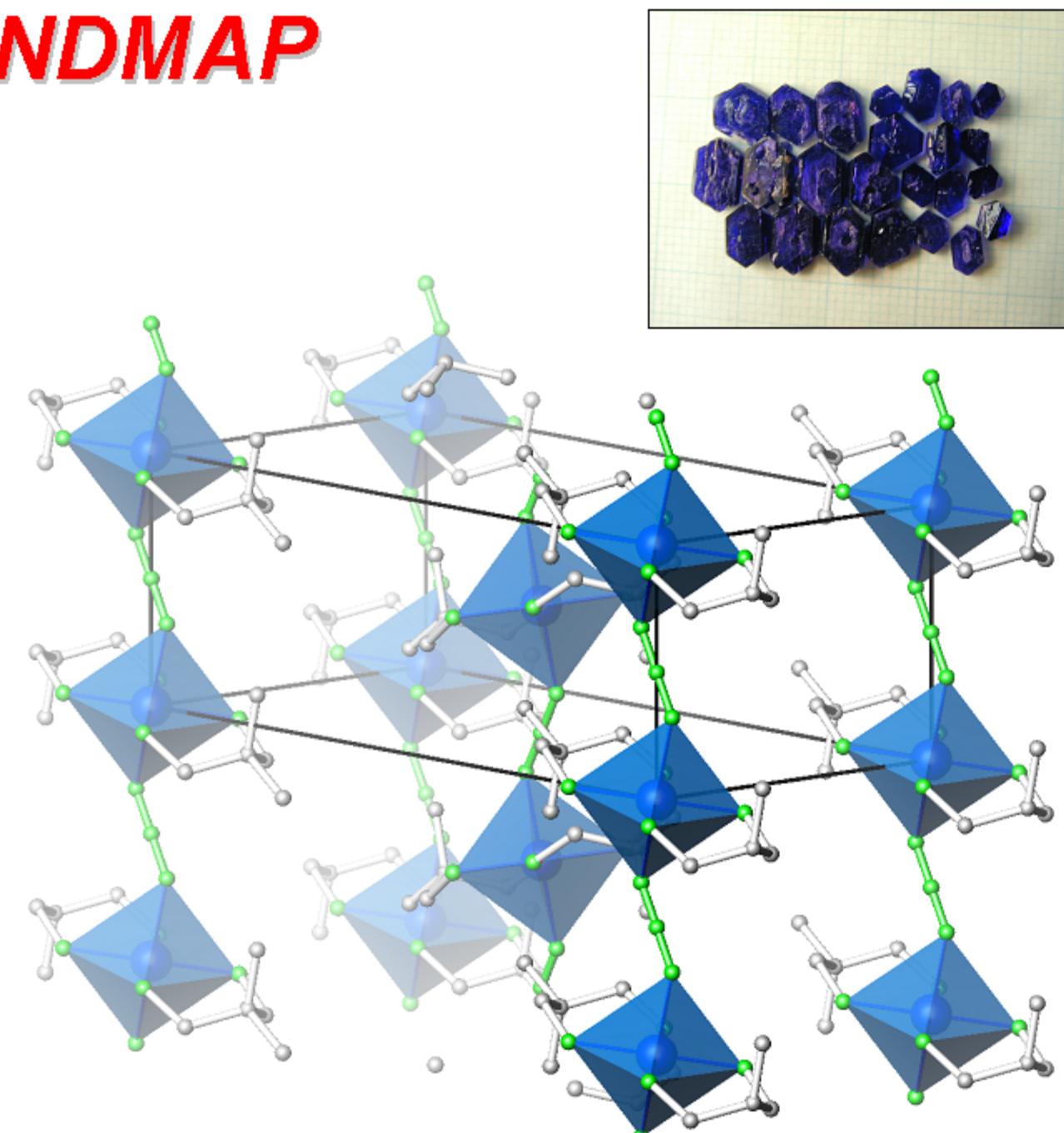
### Broken axial symmetry



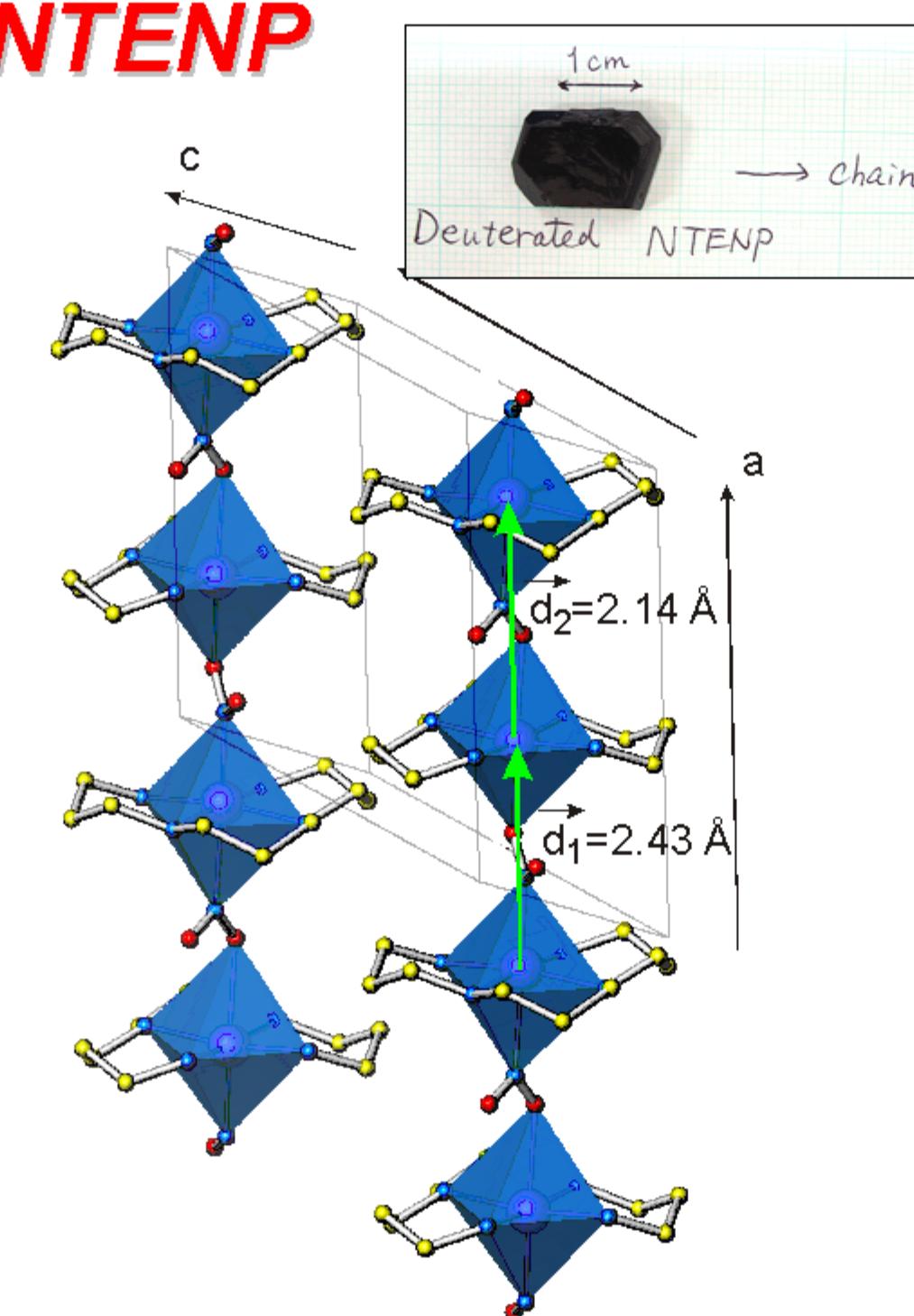
- The Haldane and dimer ground states differ by “hidden” symmetries.
- This difference is very subtle and not directly observable.
- Can there be any qualitative differences in excitations?

## Model materials

### NDMAP



### NTENP



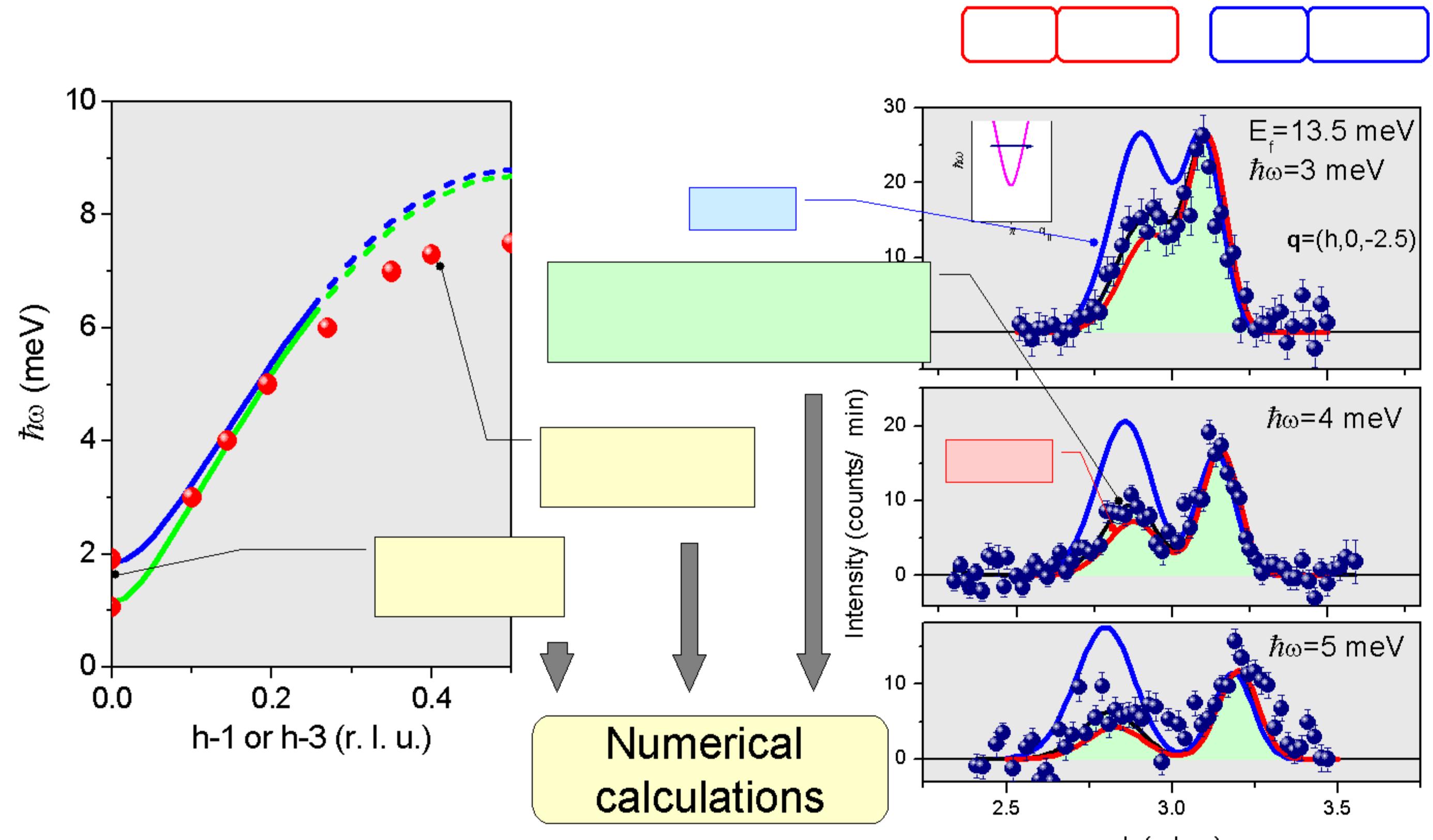
- Uniform S=1 chains: Haldane gap
- $\Delta=0.95$  meV
- Easy-plane anisotropy  $D/J \sim 0.3$
- $J_\perp/J < 10^{-3}$

- Alternating S=1 chains
- $\delta J/J = 0.32$ : dimer gap
- $\Delta \sim 1.35$  meV
- Easy-plane  $D/J \sim 0.12$
- $J_\perp/J < 10^{-3}$

## Ground state of NTENP

- Characteristic energies

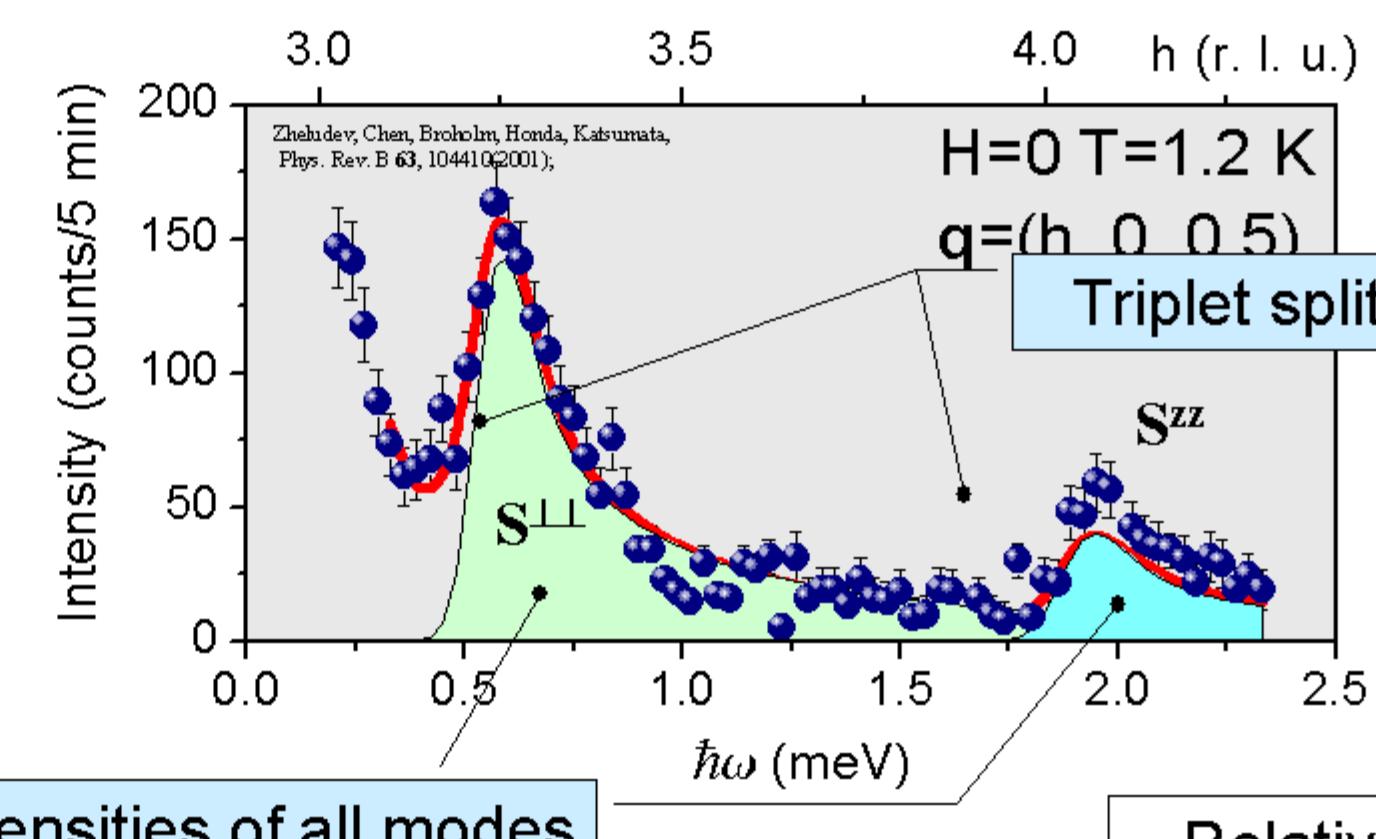
- A direct measure of dimerization



NTENP is in the dimerized phase.

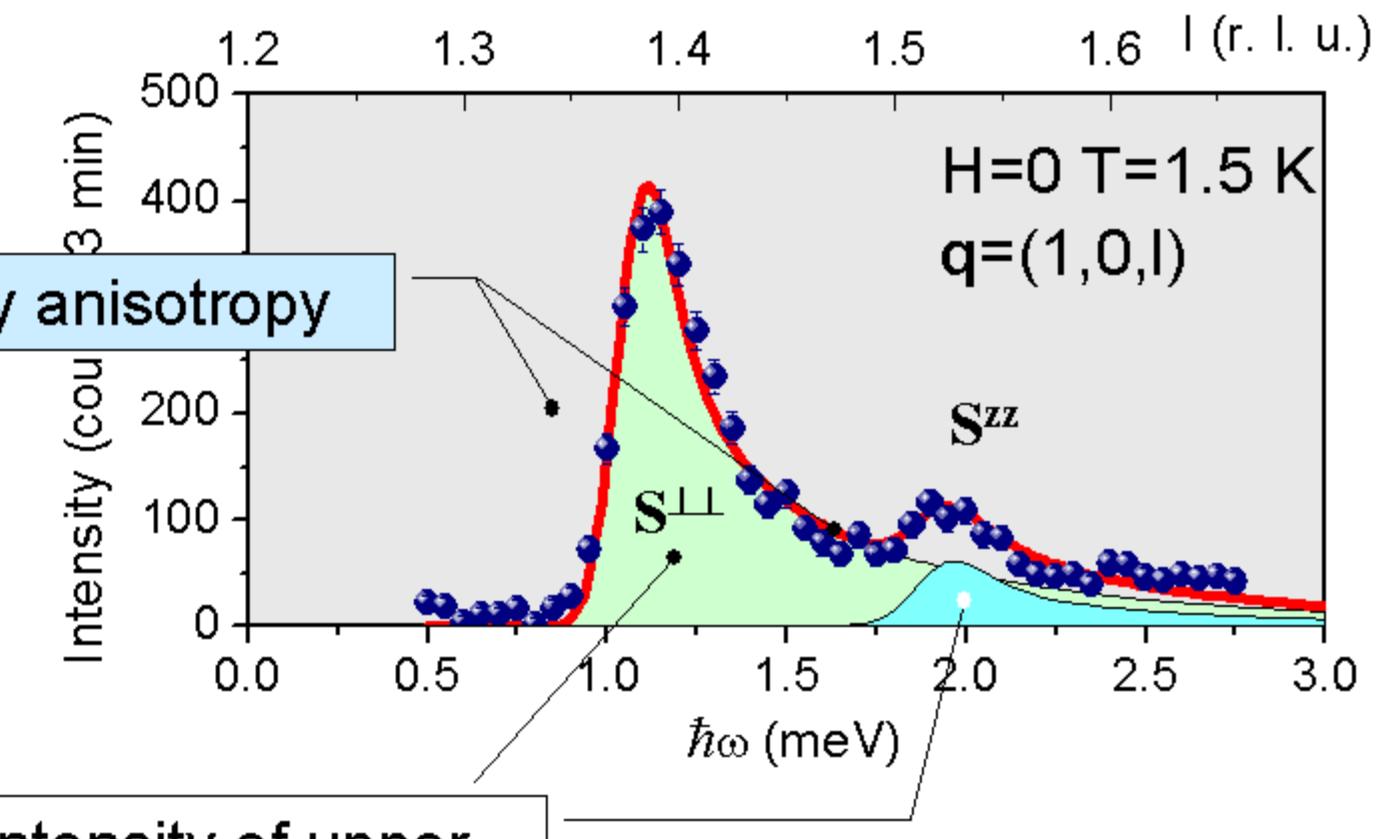
## Excitations near $q=\pi$

### NDMAP (Haldane)

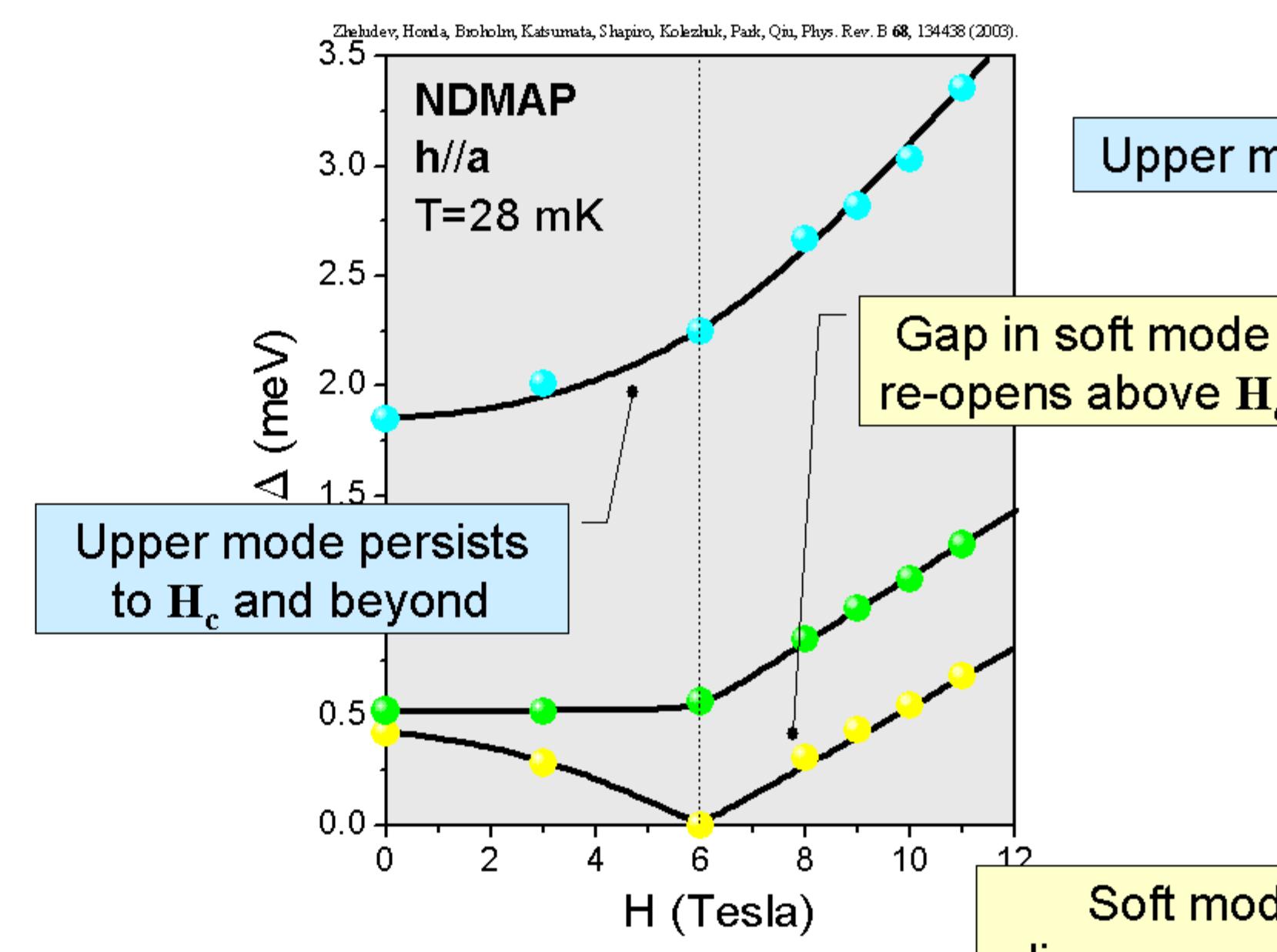


Intensities of all modes scale as  $1/\omega$

### NTENP (dimerized)

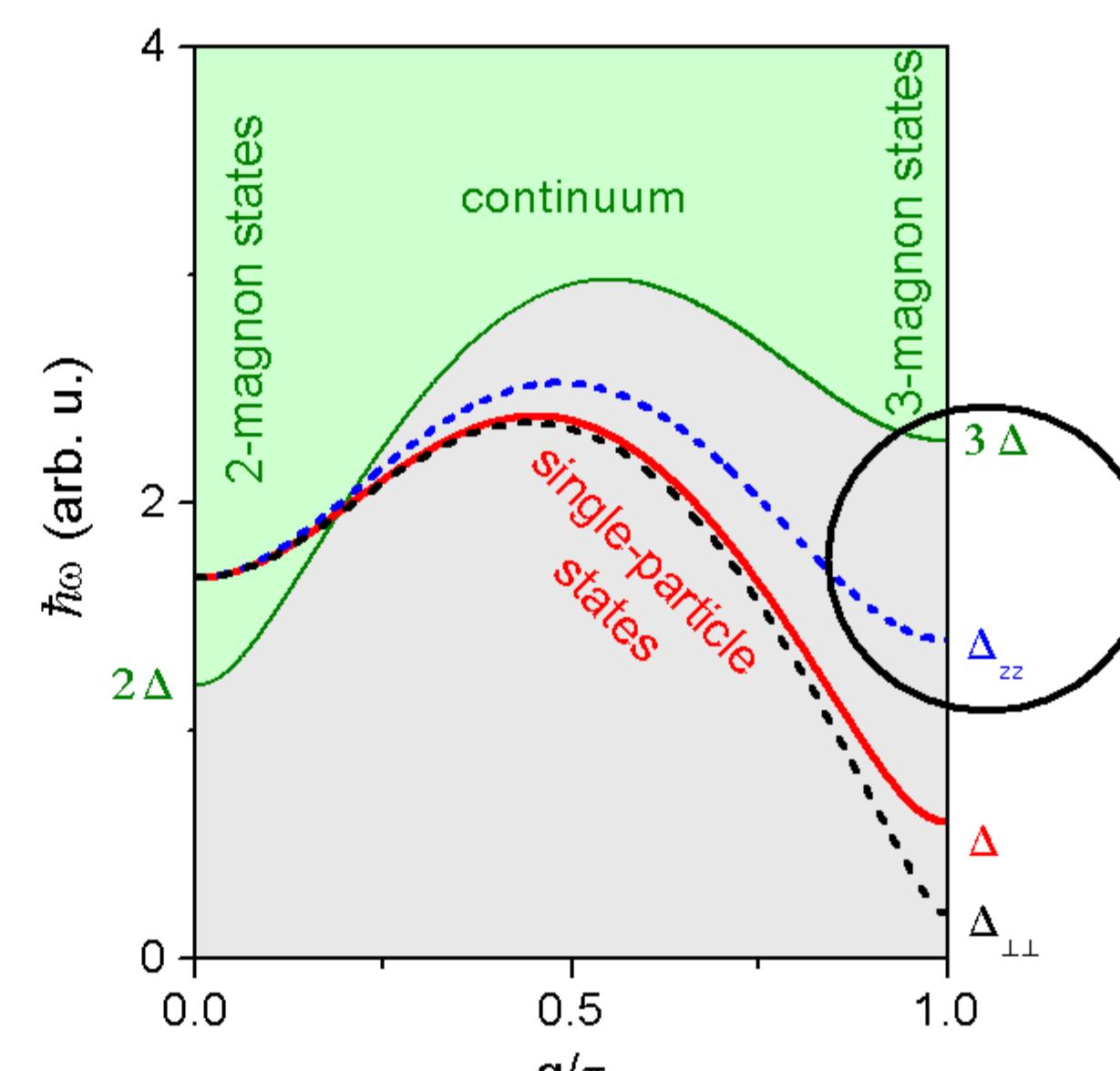


Relative intensity of upper mode is down by a factor of 3



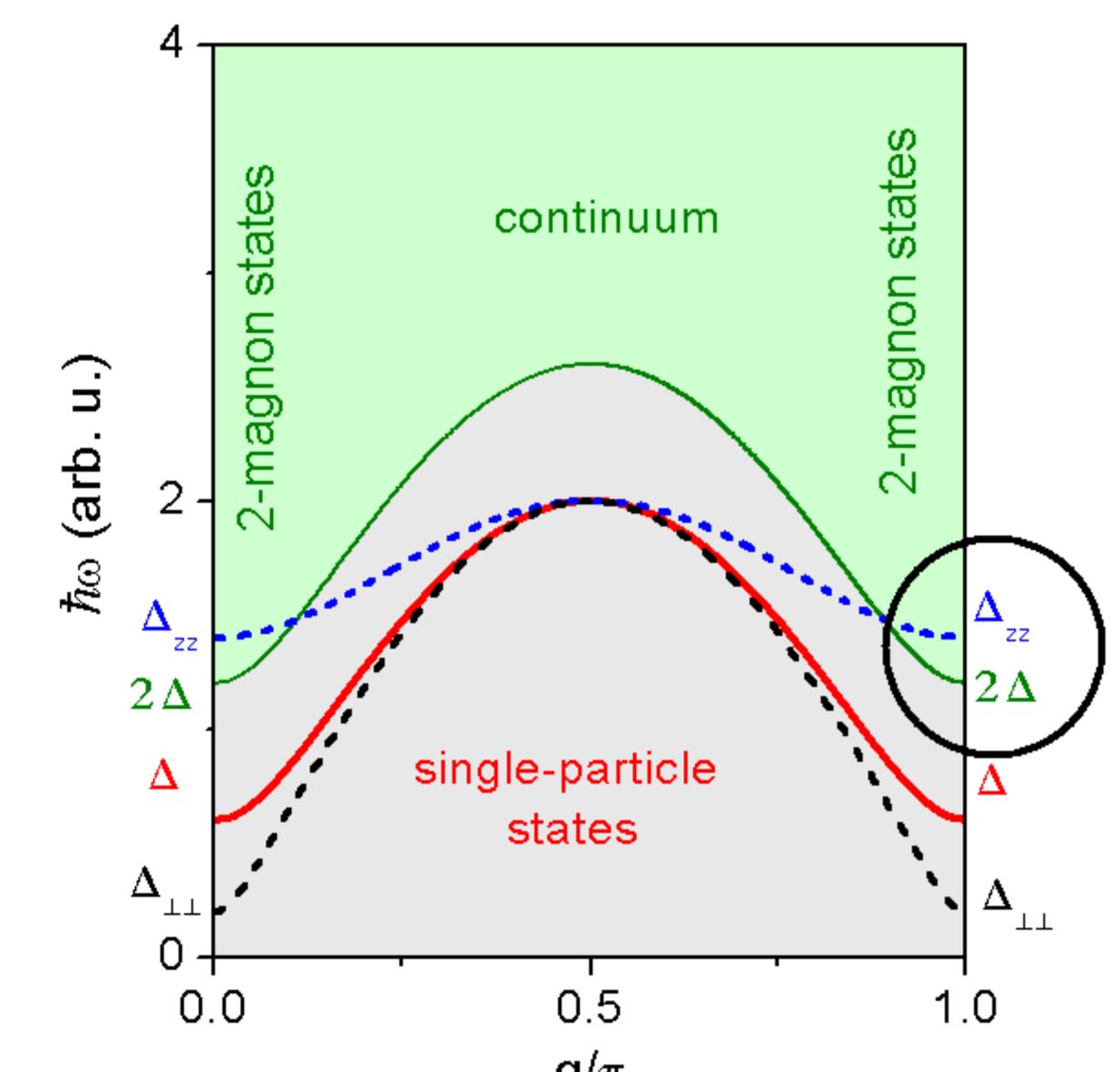
## A simple-minded picture

### Uniform (Haldane) chain



- Translational symmetry intact
- Continuum at  $q=\pi$  starts at  $3\Delta$ , above the upper mode
- Upper mode has no decay channel

### Dimerized chain



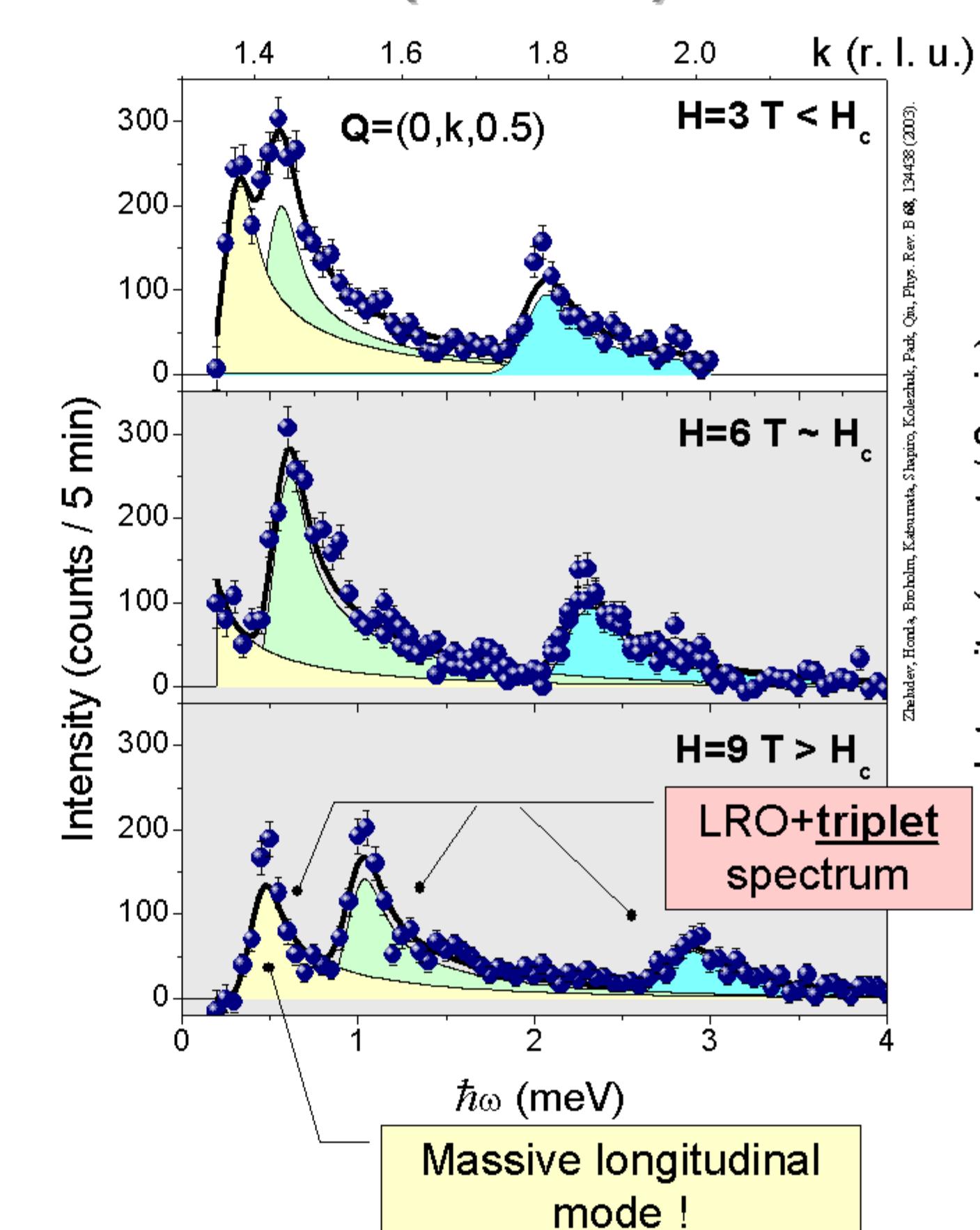
- Translational symmetry broken
- Continuum at  $q=\pi$  starts at  $2\Delta$ , below the upper mode
- Upper mode blends with continuum

Numerical analysis of size dependence of  $S^{zz}$  residue (Suga et al., 2004):

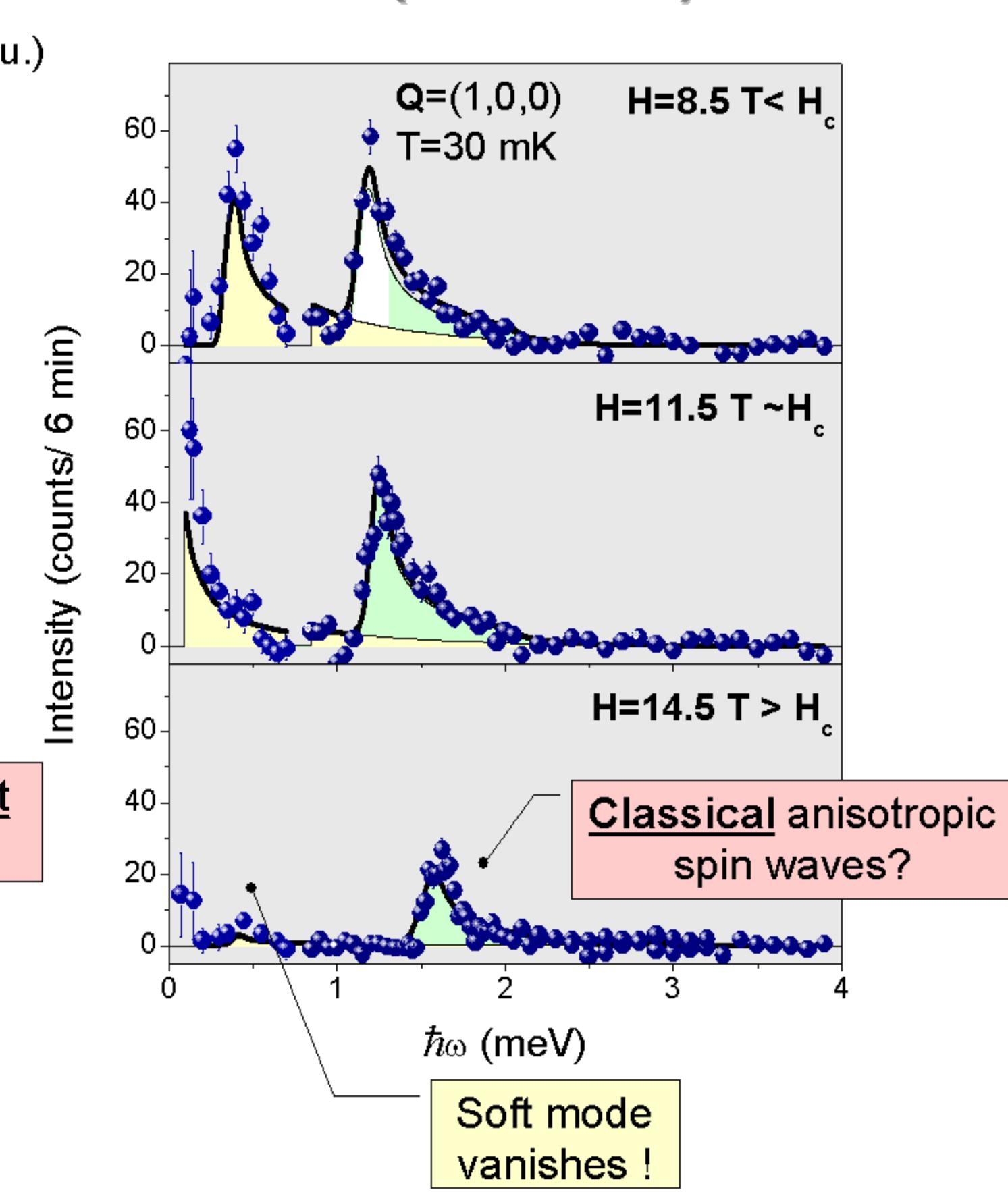
- NDMAP → at  $q=\pi$   $\Delta^{zz}$  is a single-particle pole
- NTENP → at  $q=\pi$   $\Delta^{zz}$  is the lower bound of the continuum

## Above the critical field

### NDMAP (Haldane)



### NTENP (dimerized)



## Conclusion

**Qualitatively different ground states and dynamics!**

